EUR 4963 e

COMMISSION OF THE EUROPEAN COMMUNITIES

MOLP
AN INTERACTIVE SYSTEM FOR MOLECULAR PROPERTIES CALCULATION

by

L. MONGINI and A. POLLICINI

1973

Joint Nuclear Research Centre
Ispra Establishment - Italy
Chemistry Division
and
Scientific Data Processing Centre - CETIS

LEGAL NOTICE

This report is on sale at the addresses listed on cover page 4

at the price of B.Fr. 40.—

Commission of the
European Communities
D.G. XIII - C.I.D.
29, rue Aldringen
Luxembourg
May 1973

EUR 4963 e

MOLP : AN INTERACTIVE SYSTEM FOR MOLECULAR PROPERTIES CALCULATION by L. MONGINI and A. POLLICINI

Commission of the European Communities
Joint Nuclear Research Centre — Ispra Establishment (Italy)
Chemistry Division and
Scientific Data Processing Centre — CETIS
Luxembourg, May 1973 — 22 Pages — 11 Figures — B.Fr. 40.—

An interactive system of programs for linked molecular properties calculation, realized at the CETIS computer installation in ISPRA, is described in this report.

The selection of the program sequence, the programs execution and transmission of data, are under the control of processor CARONTE. The interactive programs are used with the IBM 2250 Display Unit. The report describes the state of the system in the summer 1972.

EUR 4963 e

MOLP : AN INTERACTIVE SYSTEM FOR MOLECULAR PROPERTIES CALCULATION by L. MONGINI and A. POLLICINI

Commission of the European Communities
Joint Nuclear Research Centre — Ispra Establishment (Italy)
Chemistry Division and
Scientific Data Processing Centre — CETIS
Luxembourg May 1973 — 22 Pages — 11 Figures — B.Fr. 40.—

An interactive system of programs for linked molecular properties calculation, realized at the CETIS computer installation in ISPRA, is described in this report.

The selection of the program sequence, the programs execution and transmission of data, are under the control of processor CARONTE. The interactive programs are used with the IBM 2250 Display Unit. The report describes the state of the system in the summer 1972.

EUR 4963 e

MOLP : AN INTERACTIVE SYSTEM FOR MOLECULAR PROPERTIES CALCULATION by L. MONGINI and A. POLLICINI

Commission of the European Communities
Joint Nuclear Research Centre — Ispra Establishment (Italy)
Chemistry Division and
Scientific Data Processing Centre — CETIS
Luxembourg May 1973 — 22 Pages — 11 Figures — B.Fr. 40.—

An interactive system of programs for linked molecular properties calculation, realized at the CETIS computer installation in ISPRA, is described in this report.

The selection of the program sequence, the programs execution and transmission of data, are under the control of processor CARONTE. The interactive programs are used with the IBM 2250 Display Unit. The report describes the state of the system in the summer 1972.

EUR 4963 e

COMMISSION OF THE EUROPEAN COMMUNITIES

M O L P
AN INTERACTIVE SYSTEM FOR MOLECULAR PROPERTIES CALCULATION

by

L. MONGINI and A. POLLICINI

1973

Joint Nuclear Research Centre
Ispra Establishment - Italy
Chemistry Division
and
Scientific Data Processing Centre - CETIS

ABSTRACT

An interactive system of programs for linked molecular properties calculation, realized at the CETIS computer installation in ISPRA, is described in this report.

The selection of the program sequence, the programs execution and transmission of data, are under the control of processor CARONTE. The interactive programs are used with the IBM 2250 Display Unit. The report describes the state of the system in the summer 1972.

KEYWORDS

FORTRAN
C CODES
M CODES
COMPUTER CALCULATIONS
MOLECULAR STRUCTURE
MOLECULES
ELECTRON SPIN RESONANCE
ATOMS

MOLP : AN INTERACTIVE SYSTEM FOR MOLECULAR PROPERTIES CALCULATION

L. MONGINI and A. POLLICINI

1. INTRODUCTION

For the molecular properties calculation it is often necessary to execute a sequence of various linked computer programs; that is, a sequence in which the results of a program are used as input for a following one.

In this case it is useful to dispose of a library of programs and of a processor able to select the programs of the sequence, to control the sequence execution and to supervise the transmission of data. With such a system is possible in fact that both the number of programs inserted in the library, and also the number of allowed sequences remain open ended.

For these reasons in the computer installation of CETIS in Ispra the realization of a system of programs, useful for the molecular properties calculation, has been started. For such a system the selection of the programs of the sequence, the programs execution and transmission of data are under the control of the processor CARONTE [1] , written for IBM 360 and 370 series.

We describe in this report the state of the system in the summer of 1972; obviously the basic philosophy and the mode of use not in any way changed by the introduction of new programs. The system include at that moment the following programs :

STARTLC
* MB2250
MBLD
* PLOTMOL
CNINDOV
* SPIN
* ESR2250
CALCPLOT

The programs with an asterisk are interactive and apt to be used with the IBM 2250 Display unit. By this way the realization of a sequence of programs is possible, where all the input data can be introduced from the 2250 unit, and the output can appear on the screen of the same unit.

The data can be restricted to some information about the structure of the molecule. Starting from these data the system calculates the molecular coordinates and then the energies, the dipolar moments, the electron densities and spin densities. These last data can be used for the theoretical reconstruction of E.S.R. spectra.

Obviously, with the addition of new programs to the library, different approximation levels will became possible and also the calculation of other molecular properties.

We will now describe the processor for the automatic control of linked calculation and afterwards the programs (with greater emphasis on the programs not already described) and the flow of operations.

2. The automatic control of linked calculations

To supervise the automatic execution of the sequence of programs, the processor Caronte conceived and realized at CETIS in 1969 [1] has been chosen. The main advantage of the Caronte system is that for a class of programs to be inserted in the Caronte Program Library, data transfers between programs do not have to be classified in fixed formats. Consequently, no significant modifications have to be made to a program because its input data and output results do not have to be standardized in any way. They have only to be grouped in numbered sets of data called "Interfaces", which will be transferred, under the Caronte system control, to and from a Datapool stored in an auxiliary memory. Because of this, the Interfaces stored in the Datapool by a given program may have to be mixed and elaborated to serve as an input Interface to a program that follows. These operations are perfomed, following the wishes of the user, by Linking Routines which run under Caronte control, and which are set up for each field of application. The possibility of relying on Linking Routines for the elaboration of Interfaces has been shown to be extremely advantageous, since it allows programs to be used in the Program Library with a minimum of modification to the programs.

Two or more Interfaces belonging to different programs are said to have the same "interface number" when they contain the same kind of data, which has been written in the same way. The Linking Routine operates on one or more "interfaces" to produce another "interface" and are automatically called by Caronte.

Let us consider now the utilisation of the processor Caronte in our case. We use at the moment the version 2 of Caronte with some modifications for the definition of the sequence through the 2250 UNIT.

3. Flow of operations and interfaces description

The fig 1 shows a possible scheme of program sequence together with the interfaces and linking routines.

Every module during the job execution uses and produces some interfaces which in the scheme of fig 1 are distinguished by numbers. Equal interfaces have the same number.

We give now a concise description of the data contained in the interfaces generated during the execution of the sequence descripted in fig 1.

INTERFACES DESCRIPTION

INTERFACE 1: (1 record variable length)

- 1	Fullword	Integer	NALARM	Error indicator
- 1	"	"	M	Number of atoms
- 1	"	"	CHARGE	Total charge of the molecule
- 1	"	"	MULTIP	Total spin multiplicity of the molecule

followed by M groups, so defined:

- 1	Fullword	Integer	AN(I)	Atomic number of I^{th} atom
- 1	"	EBCDIC	EL(AN(I))	Chemical symbol " "
- 1	"	Real	C(I,1)	X-coordinate of " "
- 1	"	Real	C(I,2)	Y-coordinate of " "
- 1	"	Real	C(I,3)	Z-coordinate of " "

INTERFACE 2: (2 records)

First record variable length:

- 1	Fullword	Integer	NATOMS	Number of atoms
- 1	"	"	CHARGE	Total charge of the molecule
- 1	"	"	MULTIP	Total spin multiplicity of the molecule

followed by NATOMS elements, so defined:

- 1	Fullword	Integer	AN(I)	Atomic number of I^{th} atom

Second record variable length, formed by NATOMS groups, so defined:

- 1	Doubleword	Real	C(I,1)	X-coordinate of I^{th} atom
- 1	"	"	C(I,2)	Y-coordinate of " "
- 1	"	"	C(I,3)	Z-coordinate of " "

INTERFACE 3: (1 record fixed length)

- 18	Fullwords	EDCDIC	TITLE	Title of the case
- 1	Fullword	Integer	KNT	Counter of the cycles
- 1	"	"	ISP	Input option for interactive programs
- 1	"	"	NALARM	Error indicator
- 1	"	Real	OFF	Loop exit condition

INTERFACE 4: (2 records)

First record variable length:

- 1	Fullword	Integer	NATOMS	Number of atoms

followed by NATOMS groups, so defined:

- 1	Fullword	Integer	AN(I)	Atomic number of I^{th} atom
- 1	"	EBCDIC	EL(AN(I))	Chemical symbol " "

Second record variable length, formed by NATOMS elements, so defined:

- 1	Doubleword	Real	SPINDS(I)	S orbital spin density

INTERFACE 5: (several records)

First records variable length:

- 1	Fullword	Real	FACTL	Length conversion coefficient (cm/gauss)
- 1	"	Integer	IND	Number of elementar ESR components

followed by 1 group, so defined:

- IND	Fullwords	Real	COMPNT(I)	Factor depending on isotopic abundance of each elementar ESR component

IND records variable length, each with the following lay-out:

- 1	Fullword	Integer	LEI	Ordering number of considered elementar ESR component
- 1	"	"	NMKD	Number of groups of equivalent nuclei

followed by NMKD groups, so defined:

- 1	Fullword	Real	SPINGR(LEI,I)	Nuclear spin value of I^{th} group
- 1	"	Integer	NMEK(LEI,I)	Number of equivalent nuclei belonging the I^{th} group
- 1	"	Real	DHEK(LEI,I)	Hyperfine splitting constant of I^{th} group

INTERFACE 6: (1 record fixed lenght)

- 1	Fullword	Integer	KNT	Counter of the cyoles
- 1	"	"	I6	Return error indicator
- 1	"	Real	OFF	Loop exit condition

INTERFACE 7: (several records)

First record fixed length:

- 1	Fullword	Integer	NBD	Number of bonds added by one
- 2	Fullwords	"	DUMMY	Dummy elements (*)

(NBD-1) records fixed length, each with the following lay-out:

- 1	Fullword	EBCDIC	EL1(I)	Chemical symbol of left-atom of I^{th} bond
- 1	"	"	EL2(I)	Chemical symbol of right-atom of I^{th} bond
- 1	"	Integer	LINK1(I)	Ordering number of left-atom bonded with I^{th} bond
- 1	"	"	LINK2(I)	Ordering number of right-atom bonded with I^{th} bond
- 1	"	EBCDIC	BDTYPE(I)	Type of I^{th} bond

INTERFACE 8: (3 records)

First record fixed length:

- 1	Fullword	Integer	NALARM	Error indicator
- 1	"	"	NATOMS	Number of atoms
- 1	"	"	NBONDS	Number of bonds
- 1	"	Real	TOP	Maximum length of coordinates

Second record variable length, formed by NATOMS groups, so defined:

- 1	Fullword	EBCDIC	SYMBOL(I)	Chemical symbol of I^{th} atom
- 1	"	Real	X(I)	X-coordinate " " "
- 1	"	"	Y(I)	Y-coordinate " " "
- 1	"	"	Z(I)	Z-coordinate " " "

Third record variable length, formed by NBONDS groups, so defined:

- 1	Halfword	Integer	JJ(I)	Ordering number of left-atom bonded with I^{th} bond
- 1	"	"	KK(I)	Ordering number of right-atom bonded with I^{th} bond
- 1	"	"	LTYPE(I)	Type indicator of I^{th} bond

INTERFACE 9: (1 record fixed length)

- 1	Fullword	Integer	KNT	Counter of cycles
- 2	Fullwords	"	DUMMY	Dummy elements (*)

(*) The dummy elements are necessary to reach the smallest length (18 bytes) for 1 record to be write on direct access device.

4. Program description

4.1. STARTLC. This program is required from CARONTE at the beginning of a sequence containing a loop. STARTLC generates the interface N. 3 and also the End of File at the beginning of the data sets on the logic units 9 and 11. In these data sets, in the exemple of fig. 1, are stored the information for plotting the spectra calculated by ESR2250.

4.2. MB2250. This is the MBLD (Standard Geometric Models and Cartesian Coordinates of Molecules) [2] modified for the utilisation with IBM 2250 display unit and insertion in Caronte Library.

This program, from a minimal set of data, which in the actual version can be completely given by 2250 unit, calculates the cartesian coordinates of all atoms in the molecules. All the bonding information necessary for the definition of a molecule are given by drawing on the cathodic ray tube the structure of the molecule.
After these information some options are available and chosen by light pen. These options are useful if the operator wishes to modify the standard values of bond lengths and angles. Once calculated, the coordinates appear on the screen. At this point, three options are given to the operator:
1) to continue by sending the coordinates to the Datapool;
2) to correct some values before continuing;
3) if he realize that a mistake has been made, he can go back to the beginning of the program and give new input data.

In fig. 4 the input for the Ethyl Radical on the creen of the 2250 Unit is shown.

4.3. PLOTMOL. The program generates an isometric rapresentation of the molecule structures having in input the cartesian coordinates of atoms and some information about the bonds.

The structure performs a first rotation around the vertical axis and a second rotation perpendicular to the first one. The rotation is performed by steps, the length of which can be changed by the operator. When the total length of the rotation is arrived to 90° the movement is stopped, and restarted if required by the operator, until a full 360° rotation is completed.

During the graphic representation of the structure two interventions are possible from the operator:
a) during the rotation: to stop the movement at every moment
b) during a stop: 1) restart, 2) to modify the velocity and restart the rotation from the beginning, 3) END of the program.

4.4. CNINDOV. This program is the program CNINDO [3] which was modified in view of its inclusion in Caronte Library and was structured in overlay.
The program receives from the Datapool almost all the input data for the molecule to be calculated and in particular the coordinates calculated by MB2250.

Other data are supplied to the program through the terminal at the start of the job, as soon as the programs sequence is defined. (Figs. 2 and 3).
The program calculates, among other things, the unpaired electron densities on the different atoms of the molecule.

4.5. SPIN. Spin is a program realized for its insertion in the above described sequence. It reads from the Datapool the unpaired electron densities of the different atoms of the molecule (*) and prepares a part of the input for the successive program which effectuates the display of the E.S.R. spectra.
In particular, among other things:

a) It multiples the spin densities by the experimental magnetic nucleus constants [4] included in the program in order to obtain the distances in cm. between the peaks of the E.S.R. spectrum.
   The constants can be modified by keyboard. The average between some distances selected by operator can be calculated.
b) It recognizes the equivalent atoms (that is those giving origin to the same distances (**)) and determinates the number of groups of equivalent atoms and the number of atoms for each group. The relative probability related to the isotropic abundance is taken into account for every group.
c) It associates to nuclei with spin, the correct spin value. This value is related to the number of peaks for every group of equivalent atoms.

4.6. ESR2250. This program, already described [5], receives from the Datapool the data calculated by the program SPIN and directly from the operator some other data related to the experimental spectrum, such as the height of the spectrum, the half line width. By this way the superposition of computed and experimental spectrum became possible.
If the experimental spectrum results from more than one radical, the program can perform the addition of the component spectra. In order to do this, the computed spectra are stored on a temporary storage.

Once the display of the spectrum is obtained, the operator can choose between three possibilities: a) to modify some physical parameters of the spectrum inside the ESR2250 program; b) to start the computation from the beginning of the sequence for a different radical; c) to go out of the loop.

4.7. CALCPLOT. By this program, the vectors containing the X and Y coordinates of the spectra of which the CALCOMP plot is required, are sent back from the Data Sets 9 and 11, to the memory. The CALCOMP routines are called.

5. INPUT

We give now three different exemples of input, for the sequence described in fig. 1. All the exemples are related to the calculation of coordinates,

---

(*) more precisely the unpaired s electron densities or s orbital spin densities

(**) or Hyperfine Coupling Constants

electron densities and finally E.S.R. spectrum of Ethyl radical.

Case 1 - the input is given nearly completely by cards. The list of cards (for Job Control Language, System Caronte, and program's data) is given in the appendix 1.

Case 2 - all the data for the system CARONTE are given by cards. At the contrary, the input data for the programs are introduced through the IBM 2250 unit and substituted by a blank card. The list of cards is given in the appendix 2.

Case 3 - the data for CARONTE and programs are completely introduced from the IBM 2250 unit. The input deck is only limited to Job Control Language instructions. The list of cards is equal to the first part of appendix 2, that is until the card //SYSIN DD * (escluded).

For the input (and output) from the 2250 Unit see the figures.

6. Computing Specifications

The system of programs described in the present work is written in Fortran and partially in Assembler language for the IBM 370/165 computer and IBM 2250 Display Unit.
The 2250 Unit is used in Batch in Multi Fixed Tasks.
The memory requirements of all the System is of the order of 300 K Bytes. The total CPU time for all the program sequence for the computation and display of E.S.R. spectrum of Ethyl radical is 2 minutes. The time for permanence of the job in the partition is about 20 minutes.
For the Graphic programming we have used the packages GSP [7] and GRAFI [8] .

7. Future Developments

We believe that this system can be extended by addition of more programs. By this way the computation of other atomic and molecular properties and also the choice between different computational methods will become possible. Besides modifications are planned in order to run the entire system by use of a different type of display unit in Time Sharing mode.

8. References

1 G. Buccari, G. Fattori, C. Mongini-Tamagnini, F. Astigiano.
"CARONTE, the Euratom modular calculational system", EUR 4779, 1972.

2 M.S. Gordon and J.A. Pople
"MBLD - Standard Geometric Models and Cartesian Coordinates of Molecules"
Program 135, Quantum Chemistry Program Exchange, Indiana University, Bloomington, Indiana.

3 Paul A. Dobosh
"CNINDO: CNDO and INDO Molecular Orbital Program", Program 141, Quantum Chemistry Program Exchange, Indiana University, Bloomington, Indiana

4 John A. Pople and David L. Beveridge
"Approximate Molecular Orbital Theory", McGraw-Hill Book Company, New York 1970, Chapter 4.3)

5 L. Mongini and C. Thonet
"A program for the theoretical reconstruction of ESR spectra", EUR 4869, 1972

6 IBM System/360 Operative System Graphic Subroutine Package (GSP),
IBM System Reference Library, GC27-6932-3.

7 A. Endrizzi
"GRAFI: A Package for Programming the IBM 2250 Display Unit",EUR 4789, 1972

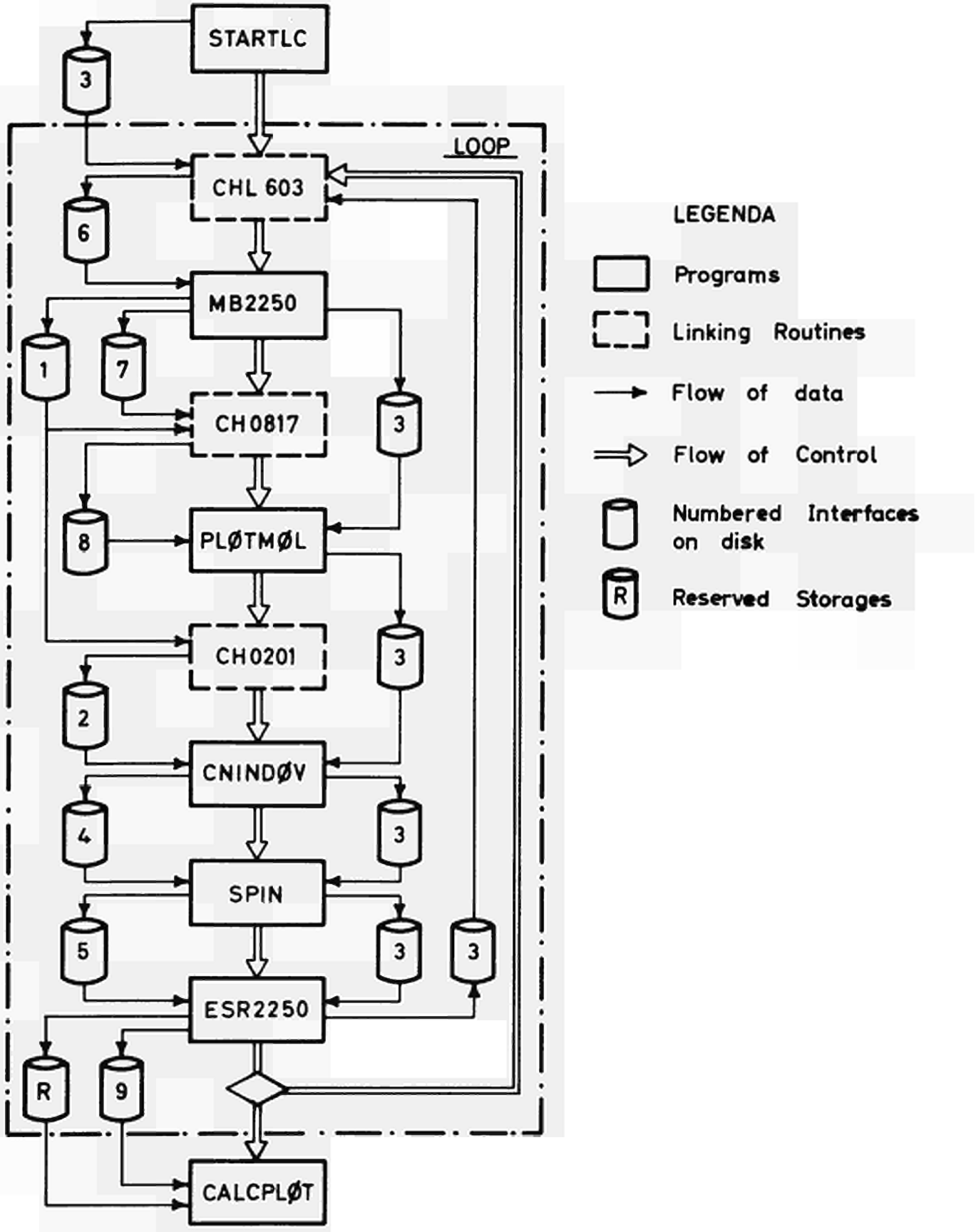


Fig. 1 - Scheme of program sequence with linking routines and interfaces

Fig. 2 - Message to the operator to require input for CNINDOV (Case 2)

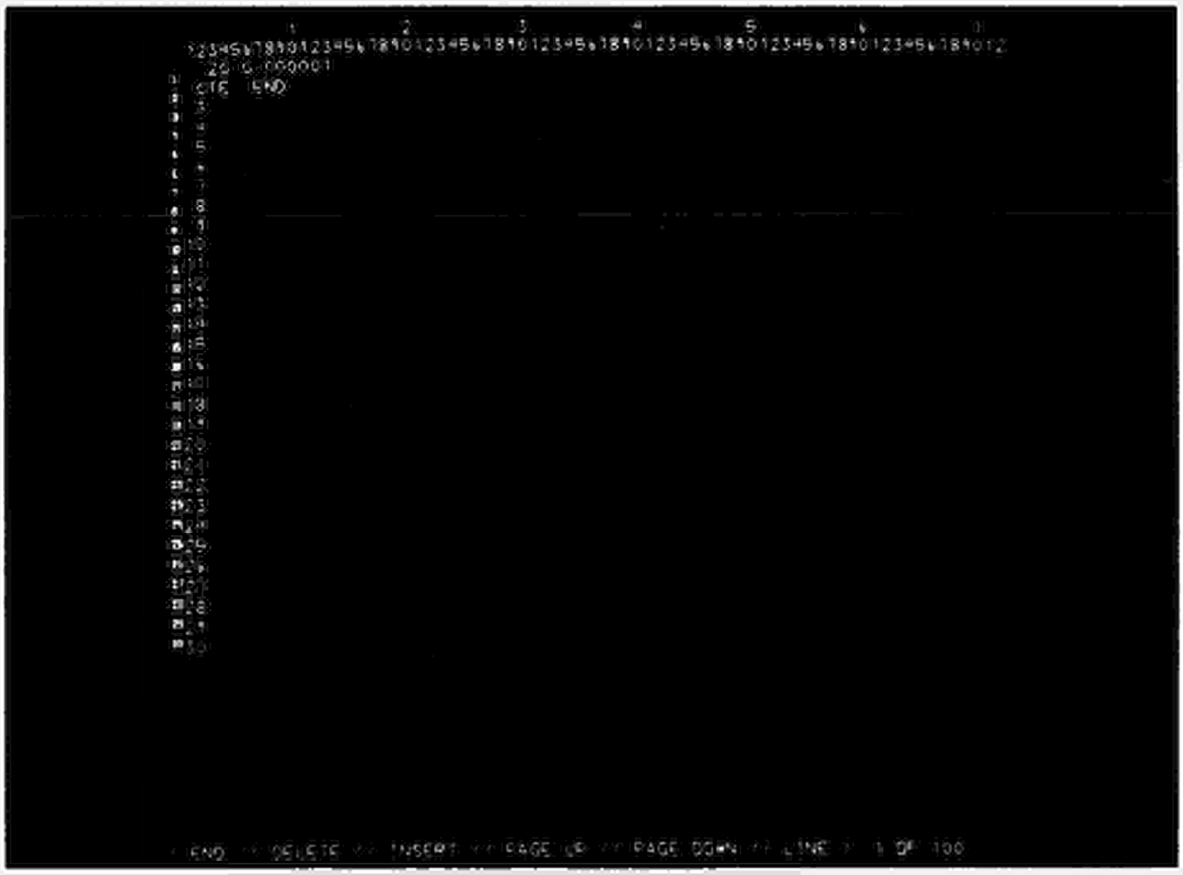


Fig. 3 - Input for CNINDOV as typed by operator

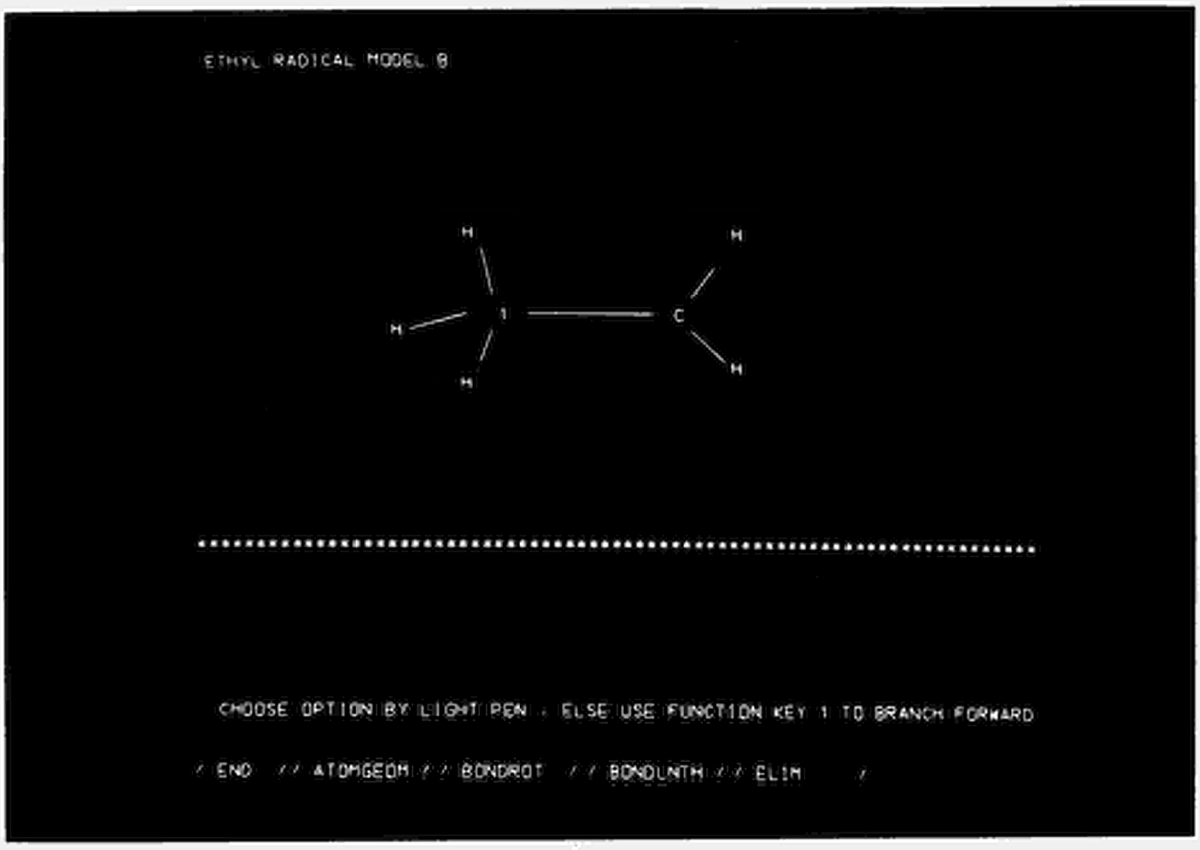


Fig. 4 - Input for MB2250.

Fig. 5 - Computed Coordinates for Ethyl Radical, as apparing on the screen.

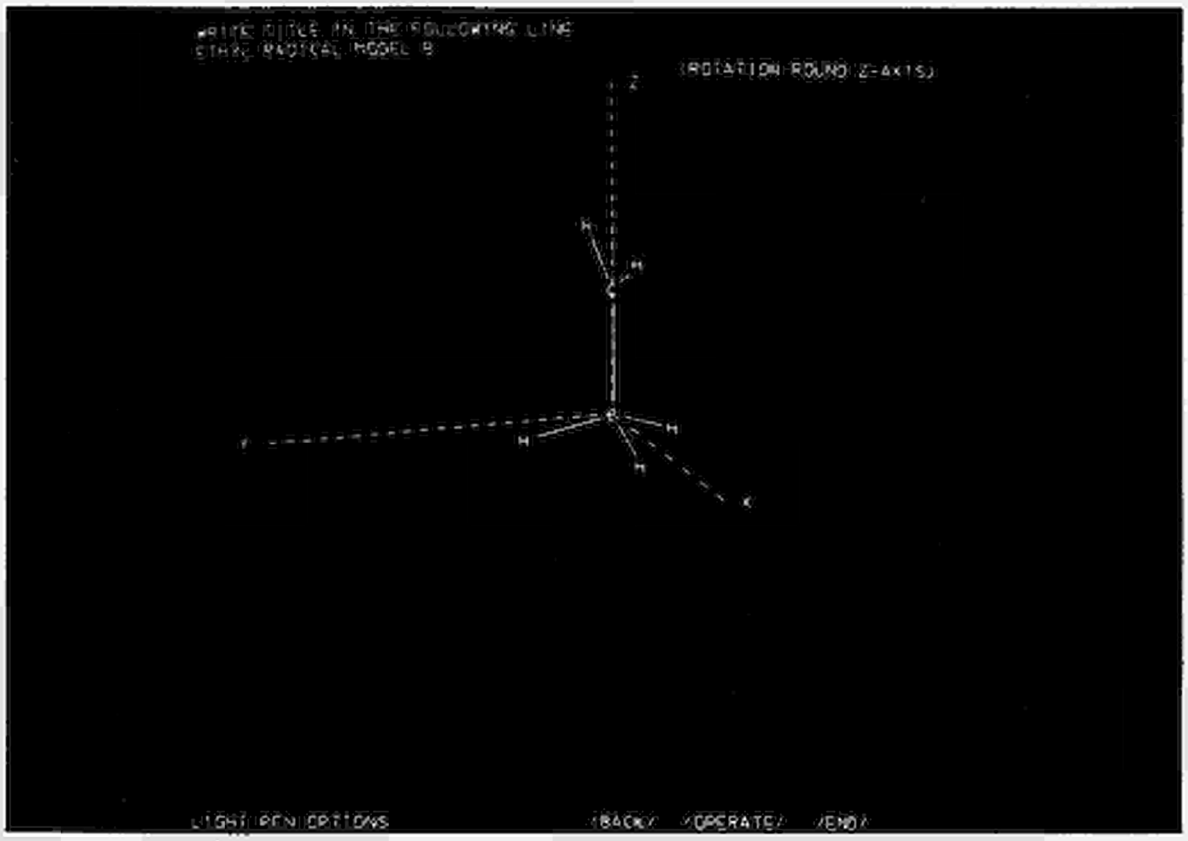


Fig. 6 - Ethyl Radical rapresentation by PLOTMOL

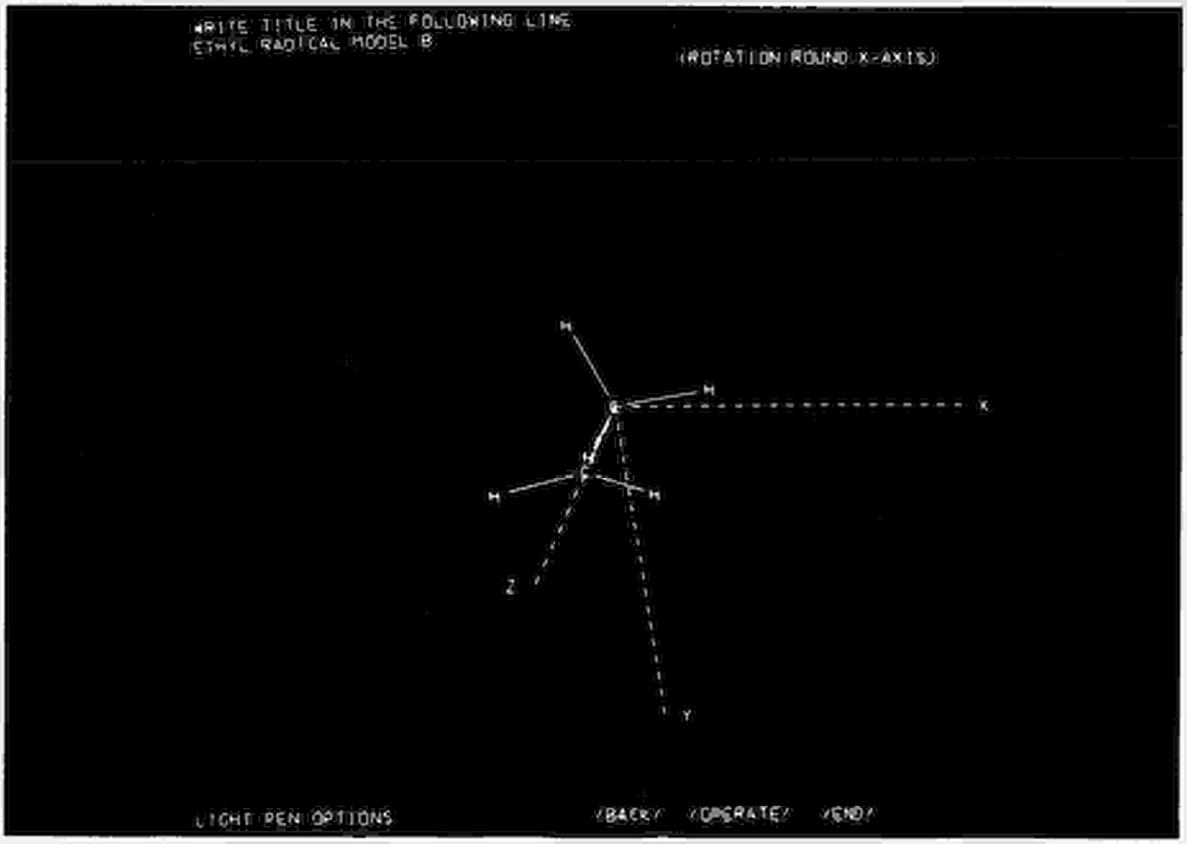


Fig. 7 - Ethyl Radical rapresentation by PLOTMOL

Fig. 8 - Input for ESR2250

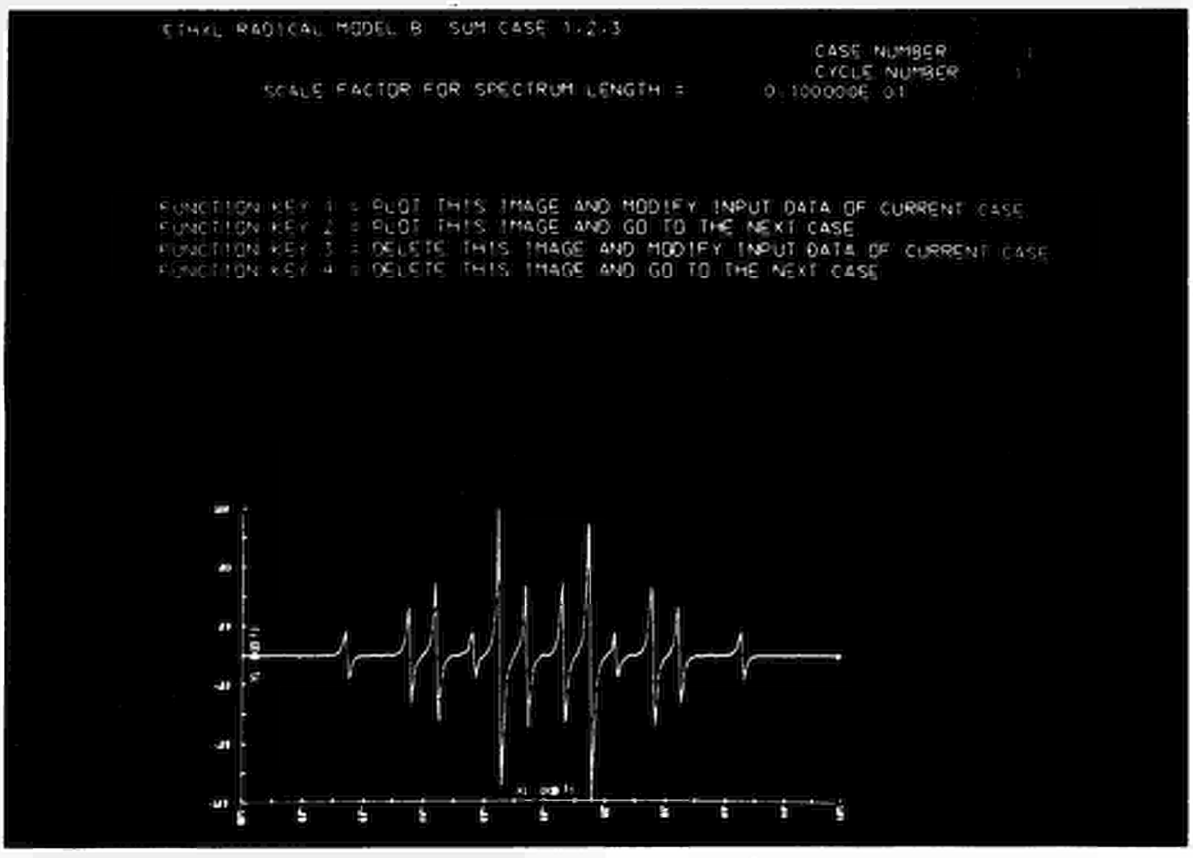


Fig. 9 - Output of ESR2250

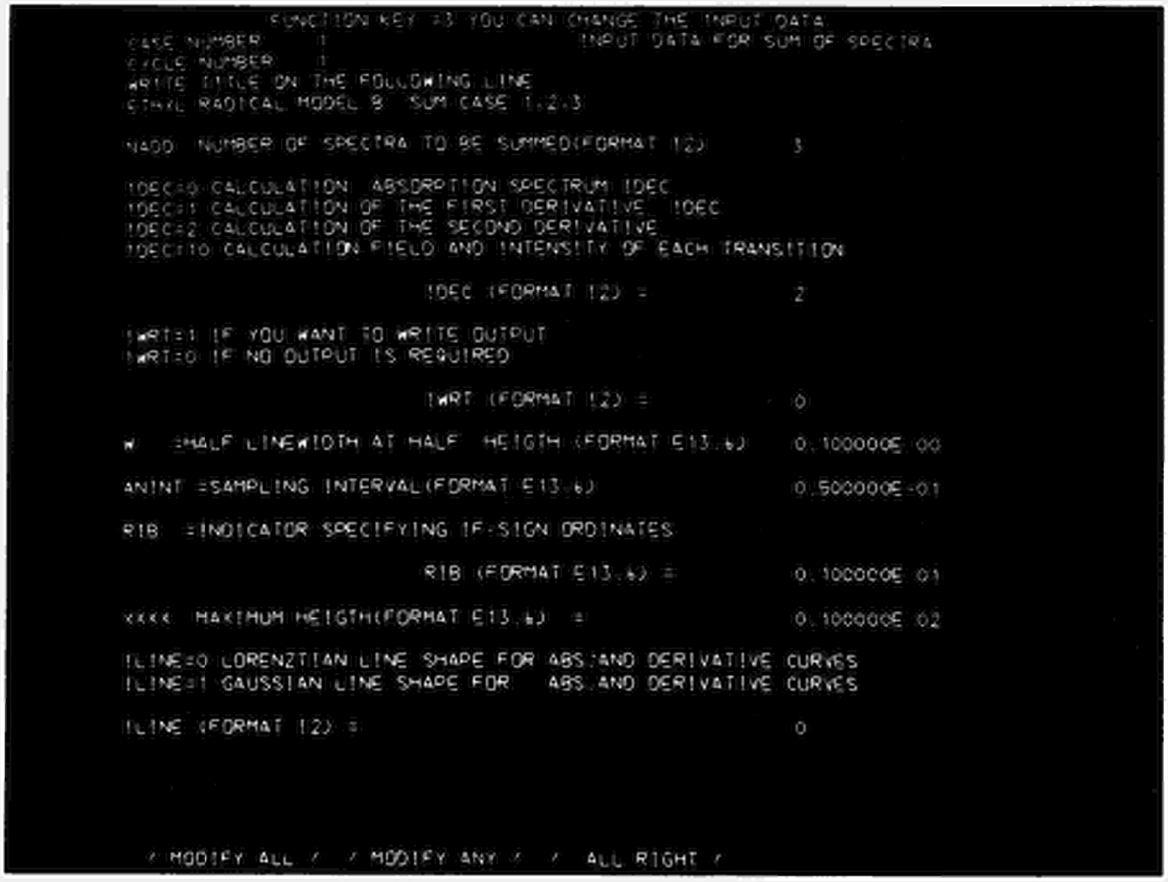


Fig. 10 - Input for ESR2250

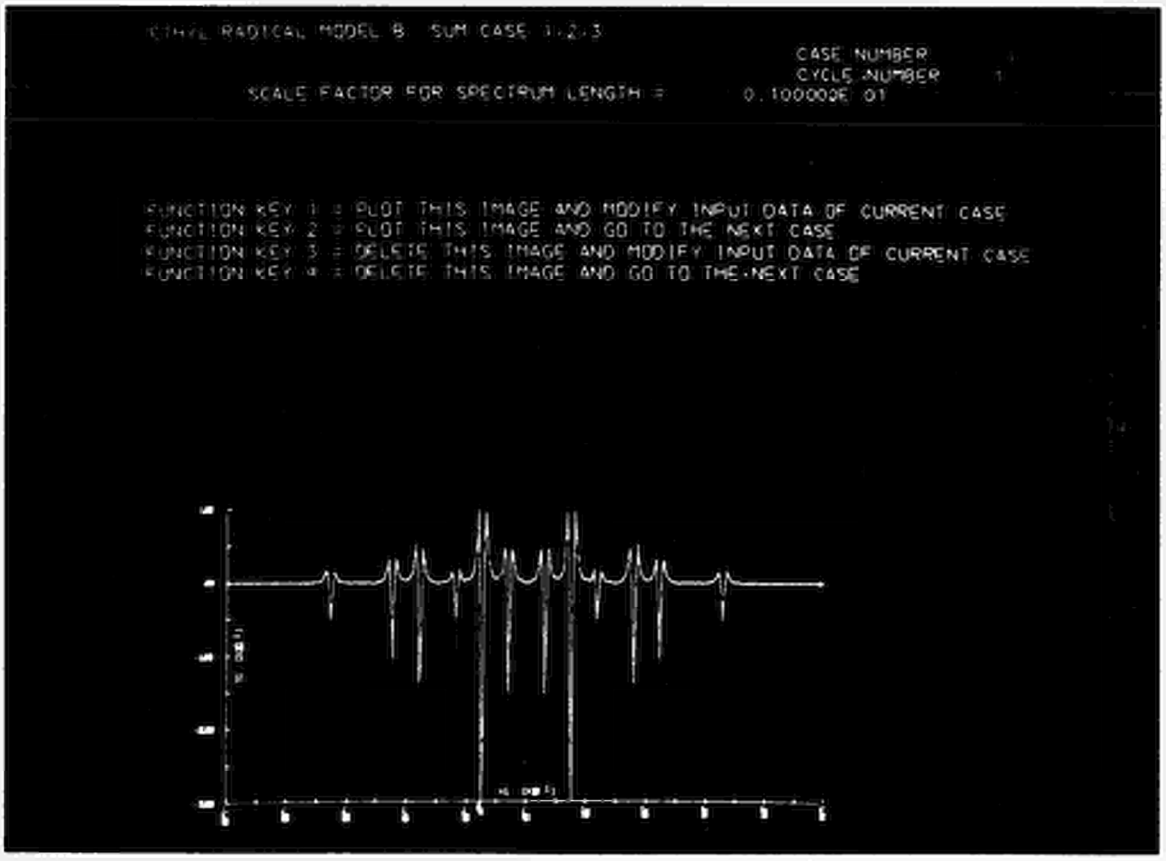


Fig. 11 - Output of ESR2250

APPENDIX 1

```
//JOBLIB    DD  DSNAME=TEMPOR,VOLUME=SER=COPIC2,UNIT=3330,DISP=SHR
//         EXEC       PGM=NUCVIDEO
//FT01F001 DD  DSNAME=HS,UNIT=3330,VOLUME=SER=COPIC1,DISP=OLD
//FT02F001 DD  DSNAME=DS,UNIT=3330,VOLUME=SER=COPIC2,DISP=OLD
//FT03F001 DD  DSNAME=LIST,UNIT=3330,VOLUME=SER=COPIC3,DISP=OLD
//FT05F001 DD  UNIT=SYSSQ,SPACE=(CYL,(5,1)),                              C
//             DCB=(RECFM=F,LRECL=80,BLKSIZE=80)
//FT06F001 DD  SYSOUT=A
//FT07F001 DD  SYSOUT=B
//FT09F001 DD  DSNAME=CALC,UNIT=3330,VOLUME=SER=COPIC1,DISP=OLD
//FT10F001 DD  UNIT=(2250-1)
//FT11F001 DD  DSNAME=X1Y1,UNIT=3330,VOLUME=SER=COPIC3,DISP=OLD
//FT16F001 DD  UNIT=TP9,VOLUME=(PRIVATE,SER=EU2675),DSNAME=CALC2675,      C
//             LABEL=(,,,OUT),DCB=(RECFM=VS,BLKSIZE=488,LRECL=484)
//FT91F001 DD  UNIT=SYSSQ,SPACE=(CYL,(1,1)),                              C
//             DSNAME=ROSSO9,DISP=(NEW,DELETE,DELETE),                    C
//             DCB=(RECFM=F,BLKSIZE=80,LRECL=80)
//FT92F001 DD  UNIT=SYSSQ,SPACE=(CYL,(1,1)),                              C
//             DSNAME=VIOLA9,DISP=(NEW,DELETE,DELETE),                    C
//             DCB=(RECFM=F,BLKSIZE=80,LRECL=80)
//FT93F001 DD  UNIT=3330,VOLUME=SER=COPIC3,DSNAME=CICCIC,DISP=SHR
//FT95F001 DD  DDNAME=SYSIN
//FT99F001 DD  UNIT=SYSSQ,SPACE=(CYL,(2,1)),DCB=(,RECFM=VS,BLKSIZE=800)
//CODLIBDD DD  DSNAME=TEMPOR,VOLUME=SER=COPIC2,UNIT=3330,DISP=SHR
//DATAPOOL DD  UNIT=SYSSQ,SPACE=(CYL,(2,2))
//LIBCODDD DD  DSNAME=CTE.CODE.LIBCH,DISP=SHR
//PCGETAB  DD  UNIT=SYSSQ,SPACE=(CYL,(1,1))
//PROGDATA DD  UNIT=SYSSQ,SPACE=(CYL,(1,1))
//PTVCORRS DD  DSN=CTE.CODE.PTCH,DISP=SHR
//TVCORRSP DD  DSN=CTE.CODE.TCCH,DISP=SHR
//WRITENT  DD  UNIT=SYSSQ,SPACE=(CYL,(1,1))
//WRITEPNT DD  UNIT=SYSSQ,SPACE=(CYL,(1,1))
//SYSABEND DD  SYSOUT=A
//SYSPRINT DD  SYSOUT=A
//SYSIN    DD  *
.CTE   BEGIN
 SQ    STARTLC-1,(MB2250-1,PLOTMOL-1,CNINDOV-1,SPIN-1,ESR2250-1),
     1CALCPLOT-1
.CTE   DATA TRANSMISSION
       MB2250-1(6) FROM STARTLC-1(3)
       PLOTMOL-1(3) FROM MB2250-1(3)
       PLOTMOL-1(8) FROM MB2250-1(1),MB2250-1(7)
       CNINDOV-1(3) FROM PLOTMOL-1(3)
       CNINDOV-1(2) FROM MB2250-1(1)
       SPIN-1(3) FROM CNINDOV-1(3)
       SPIN-1(4) FROM CNINDOV-1(4)
       ESR2250-1(3) FROM SPIN-1(3)
       ESR2250-1(5) FROM SPIN-1(5)
    L  MB2250-1(6) UNTIL DEVIATION EQUAL 1.0 FROM ESR2250-1(3)
    L  PLOTMOL-1(3) FROM MB2250-1(3)
    L  PLOTMOL-1(8) FROM MB2250-1(1),MB2250-1(7)
    L  CNINDOV-1(3) FROM PLOTMOL-1(3)
    L  CNINDOV-1(2) FROM MB2250-1(1)
    L  SPIN-1(3) FROM CNINDOV-1(3)
    L  SPIN-1(4) FROM CNINDOV-1(4)
    L  ESR2250-1(3) FROM SPIN-1(3)
    L  ESR2250-1(5) FROM SPIN-1(5)
       CALCPLOT-1(9) FROM ESR2250-1(9)
.CTE   END
.CTE   STARTLC    1
```

```
.CTE  MB2250      1
 ETHYL RADICAL    MODEL B
 0 2
 2
    C    2    H    H    H
    C    1    H    H
BONDLNTH
 1    2     1.52       TRUE
 1    3     1.09       TRUE
 1    4     1.09       TRUE
 1    5     1.09

.CTE  PLOTMOL     1

.CTE  CNINDCV     1
  20 0.000001
.CTE  SPIN        1

.CTE  ESR2250     1
           1                30          1100          1500          1500
           0                 1             0
      0.1                0.1          10.0          1.0
           0                 1             0
      0.1                0.1          10.0          1.0
           0                 1             0
      0.1                0.1          10.0          1.0
           3                 0             1                0
      0.1                0.1          10.0          1.0
      1          2       3
.CTE  CALCPLOT    1

.CTE  END
/*
```

APPENDIX 2

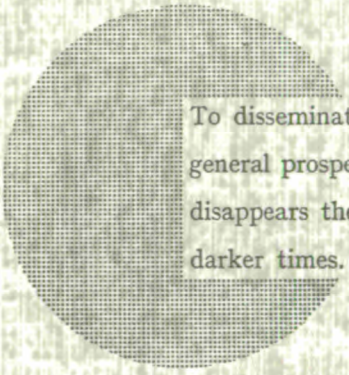
```
//JOBLIB    DD  DSNAME=TEMPOR,VOLUME=SER=COPIC2,UNIT=3330,DISP=SHR
//          EXEC      PGM=NUCVIDEO
//FT01F001  DD  DSNAME=HS,UNIT=3330,VOLUME=SER=COPIC1,DISP=OLD
//FT02F001  DD  DSNAME=DS,UNIT=3330,VOLUME=SER=COPIC2,DISP=OLD
//FT03F001  DD  DSNAME=LIST,UNIT=3330,VOLUME=SER=COPIC3,DISP=OLD
//FT05F001  DD  UNIT=SYSSQ,SPACE=(CYL,(5,1)),                              C
//              DCB=(RECFM=F,LRECL=80,BLKSIZE=80)
//FT06F001  DD  SYSOUT=A
//FT07F001  DD  SYSOUT=B
//FT09F001  DD  DSNAME=CALC,UNIT=3330,VOLUME=SER=COPIC1,DISP=OLD
//FT10F001  DD  UNIT=(2250-1)
//FT11F001  DD  DSNAME=X1Y1,UNIT=3330,VOLUME=SER=COPIC3,DISP=OLD
//FT16F001  DD  UNIT=TP9,VOLUME=(PRIVATE,SER=EU2675),DSNAME=CALC2675,       C
//              LABEL=(,,,OUT),DCB=(RECFM=VS,BLKSIZE=488,LRECL=484)
//FT91F001  DD  UNIT=SYSSQ,SPACE=(CYL,(1,1)),                              C
//              DSNAME=ROSSO9,DISP=(NEW,DELETE,DELETE),                     C
//              DCB=(RECFM=F,BLKSIZE=80,LRECL=80)
//FT92F001  DD  UNIT=SYSSQ,SPACE=(CYL,(1,1)),                              C
//              DSNAME=VIOLA9,DISP=(NEW,DELETE,DELETE),                     C
//              DCB=(RECFM=F,BLKSIZE=80,LRECL=80)
//FT93F001  DD  UNIT=3330,VOLUME=SER=COPIC3,DSNAME=CICCIO,DISP=SHR
//FT95F001  DD  DDNAME=SYSIN
//FT99F001  DD  UNIT=SYSSQ,SPACE=(CYL,(2,1)),DCB=(,RECFM=VS,BLKSIZE=800)
//CODLIBDD  DD  DSNAME=TEMPOR,VOLUME=SER=COPIC2,UNIT=3330,DISP=SHR
//DATAPOOL  DD  UNIT=SYSSQ,SPACE=(CYL,(2,2))
//LIBCODDD  DD  DSNAME=CTE.CODE.LIBCH,DISP=SHR
//PCGETAB   DD  UNIT=SYSSQ,SPACE=(CYL,(1,1))
//PROGDATA  DD  UNIT=SYSSQ,SPACE=(CYL,(1,1))
//PTVCORRS  DD  DSN=CTE.CODE.PTCH,DISP=SHR
//TVCORRSP  DD  DSN=CTE.CODE.TCCH,DISP=SHR
//WRITENT   DD  UNIT=SYSSQ,SPACE=(CYL,(1,1))
//WRITEPNT  DD  UNIT=SYSSQ,SPACE=(CYL,(1,1))
//SYSABEND  DD  SYSOUT=A
//SYSPRINT  DD  SYSOUT=A
//SYSIN     DD  *
.CTE   BEGIN
 SQ    STARTLC-1,(MB2250-1,PLOTMOL-1,CNINDOV-1,SPIN-1,ESR2250-1),
     1CALCPLOT-1
.CTE   DATA TRANSMISSION
       MB2250-1(6) FROM STARTLC-1(3)
       PLOTMOL-1(3) FROM MB2250-1(3)
       PLOTMOL-1(8) FROM MB2250-1(1),MB2250-1(7)
       CNINDOV-1(3) FROM PLOTMOL-1(3)
       CNINDOV-1(2) FROM MB2250-1(1)
       SPIN-1(3) FROM CNINDOV-1(3)
       SPIN-1(4) FROM CNINDOV-1(4)
       ESR2250-1(3) FROM SPIN-1(3)
       ESR2250-1(5) FROM SPIN-1(5)
    L  MB2250-1(6) UNTIL DEVIATION EQUAL 1.0 FROM ESR2250-1(3)
    L  PLOTMOL-1(3) FROM MB2250-1(3)
    L  PLOTMOL-1(8) FROM MB2250-1(1),MB2250-1(7)
    L  CNINDOV-1(3) FROM PLOTMOL-1(3)
    L  CNINDOV-1(2) FROM MB2250-1(1)
    L  SPIN-1(3) FROM CNINDOV-1(3)
    L  SPIN-1(4) FROM CNINDOV-1(4)
    L  ESR2250-1(3) FROM SPIN-1(3)
    L  ESR2250-1(5) FROM SPIN-1(5)
       CALCPLOT-1(9) FROM ESR2250-1(9)
.CTE   END
.CTE   STARTLC    1
```

```
.CTE   MB2250      1
.CTE   PLOTMOL     1
.CTE   CNINDOV     1        VIDEO
.CTE   SPIN        1
.CTE   ESR2250     1
.CTE   CALCPLOT    1
.CTE   END
/*
```

NOTICE TO THE READER

All scientific and technical reports published by the Commission of the European Communities are announced in the monthly periodical **"euro-abstracts".** For subscription (1 year : B.Fr. 1 025,—) or free specimen copies please write to :

Office for Official Publications
of the European Communities
Case postale 1003
Luxembourg 1
(Grand-Duchy of Luxembourg)



To disseminate knowledge is to disseminate prosperity — I mean general prosperity and not individual riches — and with prosperity disappears the greater part of the evil which is our heritage from darker times.

Alfred Nobel

SALES OFFICES

The Office for Official Publications sells all documents published by the Commission of the European Communities at the addresses listed below, at the price given on cover. When ordering, specify clearly the exact reference and the title of the document.

UNITED KINGDOM

H.M. Stationery Office
P.O. Box 569
London S.E. 1 — Tel. 01-928 69 77, ext. 365

BELGIUM

Moniteur belge — Belgisch Staatsblad
Rue de Louvain 40-42 — Leuvenseweg 40-42
1000 Bruxelles — 1000 Brussel — Tel. 12 00 26
CCP 50-80 — Postgiro 50-80

Agency :
Librairie européenne — Europese Boekhandel
Rue de la Loi 244 — Wetstraat 244
1040 Bruxelles — 1040 Brussel

DENMARK

J.H. Schultz — Boghandel
Møntergade 19
DK 1116 København K — Tel. 14 11 95

FRANCE

Service de vente en France des publications des Communautés européennes — Journal officiel
26, rue Desaix — 75 732 Paris - Cédex 15e
Tel. (1) 306 51 00 — CCP Paris 23-96

GERMANY (FR)

Verlag Bundesanzeiger
5 Köln 1 — Postfach 108 006
Tel. (0221) 21 03 48
Telex: Anzeiger Bonn 08 882 595
Postscheckkonto 834 00 Köln

GRAND DUCHY OF LUXEMBOURG

Office for Official Publications of the European Communities
Case postale 1003 — Luxembourg
Tel. 4 79 41 — CCP 191-90
Compte courant bancaire: BIL 8-109/6003/200

IRELAND

Stationery Office — The Controller
Beggar's Bush
Dublin 4 — Tel. 6 54 01

ITALY

Libreria dello Stato
Piazza G. Verdi 10
00198 Roma — Tel. (6) 85 08
CCP 1/2640

NETHERLANDS

Staatsdrukkerij- en uitgeverijbedrijf
Christoffel Plantijnstraat
's-Gravenhage — Tel. (070) 81 45 11
Postgiro 42 53 00

UNITED STATES OF AMERICA

European Community Information Service
2100 M Street, N.W.
Suite 707
Washington, D.C., 20 037 — Tel. 296 51 31

SWITZERLAND

Librairie Payot
6, rue Grenus
1211 Genève — Tel. 31 89 50
CCP 12-236 Genève

SWEDEN

Librairie C.E. Fritze
2, Fredsgatan
Stockholm 16
Post Giro 193, Bank Giro 73/4015

SPAIN

Libreria Mundi-Prensa
Castello 37
Madrid 1 — Tel. 275 51 31

OTHER COUNTRIES

Office for Official Publications of the European Communities
Case postale 1003 — Luxembourg
Tel. 4 79 41 — CCP 191-90
Compte courant bancaire: BIL 8-109/6003/200

OFFICE FOR OFFICIAL PUBLICATIONS OF THE EUROPEAN COMMUNITIES
Case postale 1003 — Luxembourg
6104